

**CS-5984 (CRN 16366)**  
**Foundations of Scientific Computing**  
**Spring 2005**

**Essential information.**

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Lecture         Mon-Wed-Fri, 9:05-9:55, 566 McBryde  
Office hours    Mon-Wed, 12-1, 632 McBryde, or by appointment  
Exam            Section 9M, May 7, 7:45-9:45  
Web Page        <http://www.cs.vt.edu/~asandu/Courses/CS5984/CS5984.html>

**Prerequisites.** Graduate standing and undergraduate course in numerical methods.

**Textbook.**

There is no single textbook for this course. Appropriate materials will be indicated in class and posted on the web.

**Topics discussed in this course include.**

- **Floating point arithmetic.** From PC's to supercomputers, all systems have special floating point hardware; compilers are called upon to optimize floating point implementations; and operating systems are designed to properly respond to floating point exceptions such as overflow. We will discuss the IEEE standard, floating point formats, rounding errors and rounding modes, floating point exceptions, and error propagation. IEEE standard, floating point formats.
- **Algorithmic errors. Accuracy of algorithms** We will discuss the basic aspects of approximation; how a continuous mathematical model is turned into a discrete model, which is suitable for computer implementation. Truncation errors, due to approximations in the mathematical formulation. Examples from interpolation and function approximation, and from discretization of differential equations.
- **Conditioning.** Some problems are more sensitive to approximation errors than others, being less amenable to computer formulations. We will talk about well and ill conditioning, error propagation, and forward and backward error analysis.
- **Stability of algorithms.** Propagation of errors through numerical algorithms and its effect on the solution. Examples from linear algebra and differential equations.
- **Cache friendly programming.** Many times scientific and engineering (floating point) models take hours, days or even weeks to complete. Can we speed up the computations while preserving the quality of the results? Sometimes a simple loop rearrangement can make a considerable impact on the code performance. Other times we need to rethink the whole computational algorithm, for example, we may look for and exploit the inherent parallelism in the problem. Examples using matrix multiplication techniques; blocking; BLAS level 1 through level 3.

- **Sparse matrices.** Specialized data structures and algorithms that exploit the special particularities of a problem can greatly enhance performance. Different representations of sparse matrices and several associated algorithms will be discussed.
- **Parallelization.** Exploiting the inherent parallelism in the problem is a powerful method to speed up the computations. We will present the task dependency graph, task interactions, and parallelization methods like domain decomposition, recursive decomposition, etc.
- **Examples.** Algorithms from linear algebra, numerical ODE's and PDE's, and mathematical software packages like BLAS and LAPACK will be used to exemplify the concepts exposed in this course.

### **Grading.**

There will be no written midterm or final examinations. Homework will be given related to the topics in class. Students will complete projects on topics to be agreed upon. Preferably the projects will be related to student's research. Students will also be required to read materials related to the course and to their research, and present them in the class.

### **Disclaimer.**

Some information given to you in class may supersede the information in this syllabus.

### **Student Complaints and Academic Misconduct.**

If you have any problems, the first step is to discuss with me directly. Should you need to speak with the Chair of the C.S. Department, you can make an appointment by speaking with the Departmental Secretary in 655 McBryde Hall.

### **Disabilities.**

Please let me know if you have a disability which requires special arrangements.